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MAGNETIC PROPERTIES OF  $R_{1-x}^{(1)}R_x^{(2)}Al_2$  ALLOYS\*

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Using the multiband  $s$ - $f$  model we derive the formulae determining the Curie temperature and magnetic moment as functions of concentration  $x$  for  $R_{1-x}^{(1)}R_x^{(2)}Al_2$  intermetallic alloys, where  $R^{(1,2)}$  denote magnetic rare earth metals. These formulae, applied to  $R_{1-x}^{(1)}R_x^{(2)}Al_2$  alloys ( $R^{(1)} = La, Lu, Y, Zr$  and  $R^{(2)} = Gd$ ) give the linear dependence of the Curie temperature and magnetic moment versus  $x$  in full agreement with experimental data.

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## 1. Introduction

The Curie temperature and magnetic moment in the paramagnetic state of  $R_{1-x}^{(1)}Gd_x^{(2)}Al_2$  samples ( $R = La, Lu, Y$ ) as functions of the concentration  $x$  ( $x \in [0, 1]$ ) have been measured in [1, 2] and more recently ( $R = Zr$ ) in [3]. A linear dependence of the Curie temperature  $T_C$  and of the magnetic moment  $M$  versus  $x$  has been found with  $T_C$  changing from zero ( $x = 0$ ) to  $T_C = 170$  K ( $x = 1$ ) and  $M$  changing from zero ( $x = 0$ ) to  $M = 7.94 \mu_B$  ( $x = 1$ ), in such a way that  $M(x)/x = 7.94 \mu_B$  ( $x \in [0, 1]$ ).

The explanation of the observed  $T_C$  behaviour of the mentioned samples (but not of the magnetic moment) has been given in the papers [4] and [2], using the formalism invented in [5, 6].

In Ref. [7] the multiband  $s$ - $f$  model has been successfully applied to explain the magnetic properties of the  $Gd(Al_{1-x}Me_x)_2$  alloys ( $Me = Cu, Ag, Pd, In, Sb, Pb, Bi, Sb, Si$ ). The method presented in [7], after some modifications, can be also successfully applied to the present case ( $R_{1-x}^{(1)}R_x^{(2)}Al_2$  alloys), where we can additionally explain the behaviour of the magnetic moment of the samples as a function of the concentration  $x$ .

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## 2. Curie temperature and magnetic moment

In Ref. [7] the Curie temperature  $T_C$  and the magnetic moment  $M$  of  $\text{GdAl}_2$  have been calculated. The corresponding formulae can be directly applied to the more general case of  $\text{RAl}_2$ , where R is a magnetic rare earth element. We recall here these formulae. The Curie temperature can be calculated from the following implicate equation:

$$T_C = \frac{S(S+1)}{3k} A, \quad (1)$$

where

$$A = \frac{5(I^{(5d)})^2 F^{(5d)}}{2W^{(5d)}} + \frac{(I^{(6s)})^2 F^{(6s)}}{2W^{(6s)}} + \frac{(I^{(3s)})^2 F^{(3s)}}{W^{(3s)}} + \frac{3(I^{(3p)})^2 F^{(3p)}}{W^{(3p)}} \quad (2)$$

$$F^{(a)} = f\left(t^{(a)} - \mu - \frac{W^{(a)}}{2}\right) - f\left(t^{(a)} - \mu + \frac{W^{(a)}}{2}\right), \quad (3)$$

$$(a = 5d, 6s, 3s, 3p)$$

$$f(z) = (\exp(\beta z) + 1)^{-1}. \quad (4)$$

In (2) the  $s$ - $f$  coupling constant has been denoted by  $I^{(a)}$  and the bandwidth of the corresponding band by  $W^{(a)}$  with the gravity centre  $t^{(a)}$ . The upper index  $a$  corresponds to  $5d$ ,  $6s$  bands of R and to  $3s$ ,  $3p$  bands of Al and  $\mu$  is the chemical potential.

The magnetic moment at  $T_C$  is given by:

$$M = 2B\sqrt{S(S+1)} \mu_B, \quad (5)$$

where

$$B = 1 + \frac{5I^{(5d)}F^{(5d)}}{2W^{(5d)}} + \frac{I^{(6s)}F^{(6s)}}{2W^{(6s)}} + \frac{I^{(3s)}F^{(3s)}}{W^{(3s)}} + \frac{3I^{(3p)}F^{(3p)}}{W^{(3p)}}. \quad (6)$$

Having in mind an alloy such as  $\text{R}_{1-x}^{(1)}\text{R}_x^{(2)}\text{Al}_2$  we have to perform the averaging procedure in (1) and (5) over the alloy configurations in order to get the equation for  $T_C$  and  $M$ . Similarly to [7] we get:

$$T_C = \frac{(1-x)S^{(1)}(S^{(1)}+1)}{3k} A^{(1)} + \frac{xS^{(2)}(S^{(2)}+1)}{3k} A^{(2)}, \quad (7)$$

$$M = 2 \left[ (1-x)B^{(1)}\sqrt{S^{(1)}(S^{(1)}+1)} + xB^{(2)}\sqrt{S^{(2)}(S^{(2)}+1)} \right] \mu_B. \quad (8)$$

The quantities  $A^{(i)} = A^{(i)}(I^{(i-5d)}, I^{(i-6s)}, t^{(i-5d)}, t^{(i-6s)}, W^{(i-5d)}, W^{(i-6s)})$  and  $B^{(i)} = B^{(i)}(I^{(i-5d)}, I^{(i-6s)}, t^{(i-5d)}, t^{(i-6s)}, W^{(i-5d)}, W^{(i-6s)})$  ( $i = 1, 2$ ) are given

by (2) and (6), respectively. The parameters for Al (3s, 3p) in  $A^{(i)}$  and  $B^{(i)}$  remain unaffected.

The equation for the chemical potential  $\mu$  of the alloy can be determined from the equation:

$$\begin{aligned} 2 \left[ (1-x) \left( \langle n_{\uparrow}^{(1-5d)} \rangle + \langle n_{\uparrow}^{(1-6s)} \rangle \right) + x \left( \langle n_{\uparrow}^{(2-5d)} \rangle + \langle n_{\uparrow}^{(2-6s)} \rangle \right) + \right. \\ \left. + \langle n_{\uparrow}^{(Al-3s)} \rangle + \langle n_{\uparrow}^{(Al-3p)} \rangle \right] = (1-x)n^{(1)} + xn^{(2)} + 6 = \\ = 6 + n^{(1)} + x(n^{(2)} - n^{(1)}), \end{aligned} \quad (9)$$

where

$$\langle n_{\uparrow}^{(i-5d,6s)} \rangle \quad (i=1, 2) \quad \text{and} \quad \langle n^{(Al-3s,3p)} \rangle$$

are the averaged occupation numbers of electrons including the band degeneracies (cf. [7]). Each of the  $R^{(i)}$  atoms ( $i=1, 2$ ) contributes  $n^{(i)}$  electrons and two Al atoms contribute  $2 \times 3 = 6$  electrons into the system, as visualized in the relation (9).

### 3. Numerical results

In order to get  $T_C = T_C(x)$  and  $M = M(x)$  we have to solve the system of implicate Eqs. (7) and (9) selfconsistently, and to calculate  $M$  from (8). We consider here the alloy  $R_{1-x}Gd_xAl_2$ , where  $R = La, Lu, Y, Zr$ . Two of them (La, Lu) are monmagnetic rare earth elements. Therefore for them  $S^{(1)} = 0$ ,  $S^{(2)} = 7/2$  (Gd) and the formulae (7) and (8) become simpler.

In Figs. 1 and 2 we show the dependence of the Curie temperature calculated from (7) and (9). We have assumed the same parameters for Al as in [7]. The parameters for Gd and La or Lu are completely irrelevant because Eq. (9) determines such a position of the chemical potential  $\mu$ , which is below the lower 5d and 6s band edges of Gd and La or Lu. In such a situation the mentioned bands are empty and therefore their contribution is zero. The magnetic moment  $M$  at  $T_C$  as a function of  $x$ , determined by (8) for  $R_{1-x}Gd_xAl_2$ , ( $R = La, Lu$ ), is a linear function of  $x$  in such a way that the ratio  $M(x)/x = 7.94 \mu_B$ , what agrees with experiments very well [1, 2]).

In the case of  $R_{1-x}Gd_xAl_2$ , where  $R$  stands for such elements as Y and Zr, the formulae (7), (8) and (9) are applicable, too. These elements are nonmagnetic ( $S^{(1)} = 0$ ,  $S^{(2)} = 7/2$  (Gd)) and their valence bands (Y:  $4d^1 5s^2$ , Zr:  $4d^2 5s^2$ ) possess the same orbital degeneracies as 5d, 6s bands of Gd, La or Lu. Also in this case the lower band edges of the 4d and 5s bands of Y and Zr lie higher than the chemical potential determined by (9). Therefore, also here, the only relevant parameters are the ones for Al. It is clear then, that the  $T_C$  dependence on  $x$  calculated from (7) and (9) gives the same results as in Figs. 1 and 2. The  $T_C = T_C(x)$  dependence seems to be universal then, for all  $R_{1-x}Gd_xAl_2$  alloys ( $R = La, Lu, Y, Zr$ ) and also the ratio  $M(x)/x = 7.94 \mu_B$ , what is the conclusion from (8). For  $R = Y$  (see

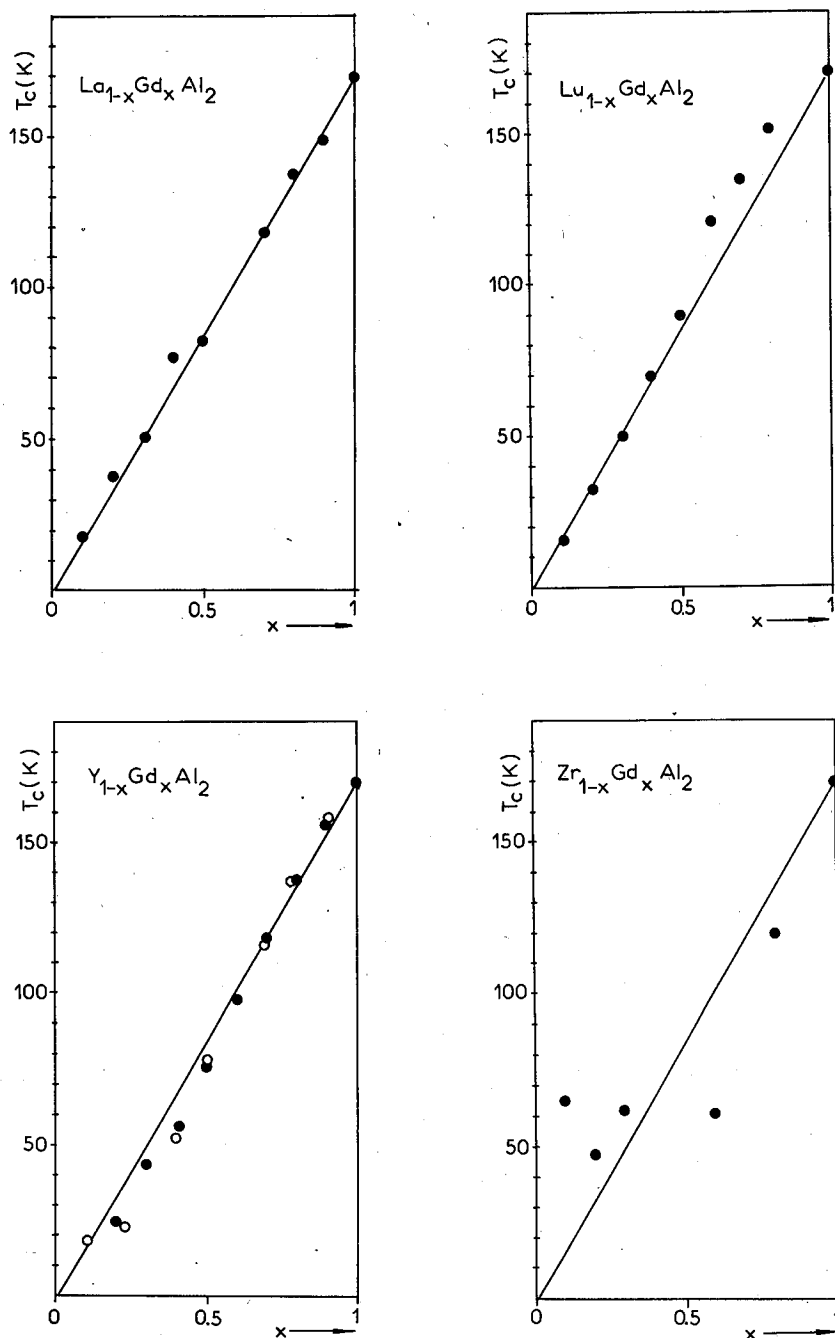


Fig. 1-4. Plot of the Curie temperature vs. concentration  $x$ , calculated from Eqs. (7) and (9). The relevant parameters in eV (only for Al) are:

$$I^{(3s)} = -0.093; \quad t^{(3s)} = 0; \quad W^{(3s)} = 4; \quad I^{(3p)} = 0.077; \quad t^{(3p)} = 2;$$

$$W^{(3p)} = 3.5; \quad n^{(1)} = 3(\text{La, Lu, Y}), \quad 4(\text{Zr}); \quad n^{(2)} = 3(\text{Gd}).$$

Fig. 3) the experimental points very closely lie to the mentioned universal linear dependence of  $T_C = T_C(x)$ , for  $R = Zr$  (Fig. 4) the agreement is, however, not so good. In the latter case the deviation from the straight line may be caused by the clusterization process in the  $Zr_{1-x}Gd_xAl_2$  samples. In our paper we have used the unperturbed density of states in a form of a rectangle for all the bands considered here ( $5d, 6s, 3p, 3d, \dots$ ). In this case the density of states is a constant in the wide energy range. When the chemical potential lies in this range for  $x \in [0, 1]$  we can obtain linear dependence of  $T_C = T_C(x)$  and  $M(x)/x = \text{const}$  only. May be, in the case of  $Zr_{1-x}Gd_xAl_2$  the unperturbed density of states in a form of rectangle is a poor approximation.

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